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On the Particle-defining Modes for a Free Neutral Scalar Field
in Spatially Homogeneous and Isotropic Universes

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Abstract

We study on the freedom in assigning Fock representations to each cosmic time for a canonically quantized free neutral scalar field in spatially homogeneous and isotropic universes. Two requirements are considered: the implementability of the Bogoliubov transformation between Fock representations at different times, and the finiteness of the energy generation rate per unit volume. We show that especially the second requirement completely determines the particle-defining modes corresponding to the Fock representations in the high frequency region for the minimal coupling case. We also show, with no assumption on the expansion law of the universes, that the scalar field should interact with the background geometry through conformal coupling in order that the Bogoliubov transformation between the Hamiltonian diagonalizing Fock representations is implementable.

1. Introduction

In the study of canonically quantized fields in expanding universes, we must construct Fock representations at each cosmic time in order to give meanings to the initial states of the quantum fields and interpret their subsequent time evolution.^{1)~7)} These Fock representations enable us to interpret the states of the quantum fields by particle language, and may play important roles in various problems; the study of the interactions of quantum fields, the statistical problems, etc.. To find a satisfactory physical principle for the construction of Fock representations in expanding universes, however, is a difficult problem and has not been solved yet.^{6), 7)}

In this paper we study this problem from a rather mathematical standpoint and try to derive constraints in assigning Fock representations to each cosmic time from some general requirements. We limit our argument to the case of a free neutral scalar field in spatially homogeneous and isotropic universes. In this case we can expand the field by the eigenfunctions of the three dimensional Laplacian and the field equation reduces to a decoupled system of second-order ordinary differential equations for functions of time, $f_k(t)$, where k denotes the eigenvalue of the Laplacian, corresponding to momentum in Minkowsky spacetime case.²⁾ Each selection of a system of solutions, $\{f_k(t)\}$, corresponds to one Fock

representation. We specify the selection at each time $t=\tau$, $\{f_{k(\tau)}(t)\}$, by giving the relation between \dot{f}_k and f_k at $t=\tau$, as $\dot{f}_{k(\tau)}(\tau) = (-i\mu_k(\tau) + \gamma_k(\tau))f_{k(\tau)}(\tau)$, with two real quantities, $\mu_k(t)$ and $\gamma_k(t)$.

In order that two Fock representations can be physically related, they must be unitary equivalent, i.e., connected by the so-called Bogoliubov transformation.³⁾ From this requirement we derive some constraints on the large- k asymptotic behavior of $\mu_k(t)$ and $\gamma_k(t)$ by examining the asymptotic behavior of the Bogoliubov transformation coefficients. The main point in this study is the expression of the Bogoliubov transformation coefficients by the WKB-type expressions for the solutions, $f_k(t)$, supplemented by the estimation of the large- k asymptotic behavior of the correction factor to the WKB approximation. This requirement, however, yields rather weak constraints on $\mu_k(t)$. Thereupon, in order to obtain stronger constraints, we next consider the energy generation rate. Though the Hamiltonian for the quantum field in a finite volume is a divergent quantity, the difference of its vacuum expectation values at two different times, referred to as energy generation rate in this paper, should be finite.^{8),9)} This is the second requirement. From this requirement $\mu_k^2(t)$ is determined up to the order of $O(1)$ in k for large k if the quantum field interacts with the background geometry through minimal coupling.

Perhaps the most natural choice of the Fock representations is the one that diagonalizes the Hamiltonian at each cosmic time.^{10),11)} Some authors, however, asserted that this choice is not adequate by showing that the Bogoliubov transformation is not implementable for some special expansion law of the universe when the coupling is minimal.^{2),12)} On the other hand it was pointed out that this trouble does not occur for a Friedmann-type universe if the coupling is conformal.¹³⁾ As a special application of our results, we clarify this point. Namely we show, with no assumption on the expansion law of the universes, that the coupling of the scalar field with the background geometry must be conformal in order that the Bogoliubov transformation between the Hamiltonian diagonalizing Fock representations is implementable, and for this choice the energy generation rate also remains finite.¹⁴⁾ Fulling has also derived the same conclusion by a similar method to ours.¹⁷⁾

The program of this paper is as follows. In § 2 we summarize some fundamental formulas on the canonically quantized free neutral scalar field and the Bogoliubov transformation, and present fundamental assumptions and notations used in this paper. In § 3 we derive the expression for the Bogoliubov transformation coefficients by the WKB-type solution of the wave equation. Then in § 4 we examine the large- k asymptotic behavior of the correction factor to the WKB approximation and apply it to the study of the constraints imposed by the implementability condition of the Bogoliubov transformation. Next we study the

energy generation rate in § 5. § 6 is devoted to concluding remarks.

2. Mode Expansion of a Canonically Quantized Free Neutral Scalar Field and the Bogoliubov Transformation

The Lagrangian density of a free neutral scalar field ϕ in a background geometry $g_{\mu\nu}$ is given by

$$\mathcal{L} = -\frac{1}{2}\sqrt{-g}\left[g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + (m^2 + \frac{\xi}{6}\mathcal{R})\phi^2\right], \quad (2-1)$$

where m is the mass of the field, \mathcal{R} is the Ricci scalar of the metric $g_{\mu\nu}$, and $\xi = 0$ and 1 for minimal and conformal coupling, respectively. The corresponding field equation is

$$\frac{1}{\sqrt{-g}}\partial_\mu(\sqrt{-g}g^{\mu\nu}\partial_\nu\phi) - (m^2 + \frac{\xi}{6}\mathcal{R})\phi = 0. \quad (2-2)$$

In a spatially homogeneous and isotropic universe whose metric is expressed as

$$ds^2 = R(t)^2(-dt^2 + d\sigma^2), \quad (2-3)$$

where $d\sigma^2$ denotes the time-independent metric of a homogeneous and isotropic three dimensional Riemannian space, we can expand the field ϕ by the complete set of eigenfunctions $\mathcal{Y}_{(k)}$ of the three dimensional Laplacian Δ_3 associated with $d\sigma^2$;

$$\Delta_3\mathcal{Y}_{(k)} = -k^2\mathcal{Y}_{(k)}, \quad (2-4)$$

where (k) denotes the set of indices which labels the eigenfunctions belonging to the same eigenvalue k .²⁾ We choose the phases of $\mathcal{Y}_{(k)}$ so that

$$\mathcal{Y}_{(k)}^* = \mathcal{Y}_{-(k)} \quad , \quad (2-5)$$

where the symbol $-(k)$ denotes some set of indices corresponding to the eigenvalue k , and normalize $\mathcal{Y}_{(k)}$ by the conditions

$$\int dv \mathcal{Y}_{(k)} \mathcal{Y}_{(k')}^* = \delta_{(k)(k')} \quad , \quad (2-6)$$

where dv is the invariant volume on the homogeneous three space, and $\delta_{(k)(k')}$ denotes the product of Kronecker deltas and/or δ -functions with respect to indices (k) . Since we do not need the details of $\mathcal{Y}_{(k)}$ in this paper, we do not write their explicit expressions.^{2),15)} With these eigenfunctions, a complete set of solutions of Eq.(2-2) is given by the functions of form $R^{-1} f_k(t) \mathcal{Y}_k$, where $f_k(t)$ satisfies the reduced field equation

$$\ddot{f}_k + \Omega^2 f_k = 0 \quad , \quad (2-7)$$

where the dot denotes d/dt , and

$$\Omega^2 = k^2 + m^2 R^2 + \xi \chi + (\xi - 1) R^{-1} \ddot{R} \quad , \quad (2-8)$$

where $\chi = 0, 1$, and 1 for spatially flat, hyperbolic, and spherical universes, respectively.

The canonically quantized free neutral scalar field is expressed by annihilation and creation operators, $a[(k)]$ and $a[(k)]^\dagger$, as follows:²⁾

$$\phi = R^{-1} \sum_{(k)} (f_{(k)} \mathcal{Y}_{(k)} a[(k)] + f_{(k)}^* \mathcal{Y}_{(k)}^* a[(k)]^\dagger), \quad (2-9)$$

$$[a[(k)], a[(k')]] = 0, \quad [a[(k)], a[(k')]^\dagger] = \delta_{(k)(k')}, \quad (2-10)$$

where f_k is a solution of Eq.(2-7) satisfying the condition,

$$\dot{f}_k \dot{f}_k^* - f_k^* \dot{f}_k = i, \quad (2-11)$$

and by $\sum_{(k)}$ integration is supposed for the continuous part of (k) . For each choice of a set of solutions of Eq.(2-7) satisfying condition (2-11), referred to as particle-defining modes in this paper, the corresponding annihilation and creation operators define a Fock representation of ϕ in the usual manner.³⁾ Since in this paper we are interested in how freely we can choose Fock representations at each cosmic time, we must assign modes $f_{k(\tau)}(t)$ to each time $t=\tau$. As mentioned in § 1, we do this by specifying $f_{k(\tau)}(t)$ by giving the relation between \dot{f}_k and f_k at $t=\tau$, as

$$\dot{f}_{k(\tau)}(\tau) = (-i\mu_k(\tau) + \gamma_k(\tau)) f_{k(\tau)}(\tau), \quad (2-12)$$

where $\mu_k(t)$ and $\gamma_k(t)$ are real functions of t and k and $\mu_k(t)$ is positive definite. From Eqs.(2-11) and (2-12) we obtain

$$|f_{k(\tau)}(\tau)|^2 = \frac{1}{2\mu_k(\tau)} \quad , \quad (2-13)$$

therefore condition (2-12) determines a solution of Eq.(2-7) up to constant phase. In the following sections we study the constraints imposed on the large- k behavior of $\mu_k(t)$ and $\gamma_k(t)$. A crucial assumption on these functions is that they depend on k monotonically for large k and the character of their asymptotic behavior is independent of t . Without this assumption we can derive no constraint on μ and γ . We regard this assumption as a stronger version of the locality in the definition of the particle-defining modes.

The Bogoliubov transformation coefficients α_k and β_k between the two Fock representations at $t=t_0$ and $t=t_1$ ^{1), 2), 8)} is defined by

$$f_{k(t_1)}(t) = \alpha_k f_{k(t_0)}(t) + \beta_k f_{k(t_0)}^*(t) \quad , \quad (2-14)$$

and from Eq. (2-11) they satisfy the condition

$$|\alpha_k|^2 - |\beta_k|^2 = 1 \quad . \quad (2-15)$$

Let $a_\tau[(k)]$ and $|\mathcal{V}_\tau\rangle$ be the annihilation operators and the Fock vacuum corresponding to the modes $f_{k(\tau)}$, respectively:

$$a_\tau[(k)] |\mathcal{V}_\tau\rangle = 0 \quad . \quad (2-16)$$

Then Eqs. (2-9) and (2-14) yield the relation

$$a_{t_1}[(k)] = \alpha_k^* a_{t_0}[(k)] - \beta_k^* a_{t_0}[-(k)]^\dagger \quad (2-17)$$

and from this and Eqs.(2-15) and (2-16) the vacuum-to-vacuum transition amplitude is given by ^{1),2)}

$$|\langle \mathcal{V}_{t_1} | \mathcal{V}_{t_0} \rangle|^2 = \prod_{(k)} |\alpha_k|^{-2} = \prod_{(k)} (1 + |\beta_k|^2)^{-1} . \quad (2-18)$$

The implementability condition of the Bogoliubov transformation between the two Fock representations, i.e., the condition the two Fock representations are unitary equivalent, is expressed as ^{1),2)}

$$0 < |\langle \mathcal{V}_{t_1} | \mathcal{V}_{t_0} \rangle|^2 < +\infty . \quad (2-19)$$

By the well-known theorem on the absolute convergence of infinite products, from Eq.(2-18), condition (2-19) is equivalent to

$$\sum_{(k)} |\beta_k|^2 < +\infty . \quad (2-20)$$

If we define the particle number N_τ by

$$N_\tau = \sum_{(k)} a_\tau[(k)]^\dagger a_\tau[(k)] , \quad (2-21)$$

we obtain the relation ¹⁾

$$\sum_{(k)} |\beta_k|^2 = \langle \mathcal{V}_{t_0} | N_{t_1} | \mathcal{V}_{t_0} \rangle . \quad (2-22)$$

The right-hand side of Eq.(2-22) represents the number of the particles generated at $t=t_1$ from the vacuum state at $t=t_0$, therefore it is, if not zero, infinite for the open universes. This is a familiar trouble associated with the infinite spatial volume and not physically essential one. We avoid this difficulty in the usual manner ¹⁾ by restricting the field in a large but finite volume, and imposing some appropriate boundary condition on it. Then, noting that the equations which determine β_k , Eqs.(2-7),(2-12) and (2-14), are all independent of the structure of the spectrum of k , hence so is β_k itself, and that the number density of modes with respect to k per unit volume is proportional to k^2 for large k regardless of κ , the implementability condition of the Bogoliubov transformation can be expressed instead of Eq.(2-20) as

$$\int_0^{+\infty} dk k^2 |\beta_k|^2 < +\infty. \quad (2-23)$$

Here we assumed that there occurs no infrared trouble since we are working in a finite volume.

3. Some Formulas for the Bogoliubov Transformation Coefficients.

In this section we derive formulas which express the Bogoliubov transformation coefficients by the correction factor to the WKB approximation for a solution of Eq.(2-7). These formulas play important roles in the study of the large- k

asymptotic behavior of α_k and β_k , and the constraints imposed on μ and γ in the following sections.

Let $X(t)$ be the solution of Eq.(2-7) satisfying the condition

$$X(t_0) = 1, \quad \dot{X}(t_0) = -i\Omega_0, \quad (3-1)$$

where Ω_0 is the value of Ω at $t=t_0$. Then $f_{(t_j)}(t)$ ($j=0,1$) are expressed by $X(t)$ as

$$f_{(t_j)} = A_j X + B_j X^*. \quad (3-2)$$

From now on the subscript k for various quantities will be suppressed. From conditions (2-12) and (2-13), we can express A_j and B_j by X as

$$A_j = \frac{e^{i\theta_j}}{2\sqrt{2\mu_j}\Omega_0} [\dot{X}_j^* + (i\mu_j - \gamma_j)X_j^*], \quad (3-3)$$

$$B_j = -\frac{e^{i\theta_j}}{2\sqrt{2\mu_j}\Omega_0} [\dot{X}_j + (i\mu_j - \gamma_j)X_j], \quad (3-4)$$

where the subscript j for the quantities in the right-hand sides represents the values estimated at $t=t_j$, and θ_j are arbitrary real numbers. From Eq.(2-14) α and β are expressed by A_j and B_j , hence by X as

$$\alpha = 2\Omega_0 [A_0^* A_1 - B_0^* B_1] = \frac{e^{i(\theta_1 - \theta_0)}}{4\sqrt{\mu_0\mu_1}\Omega_0} \mathcal{L}, \quad (3-5)$$

$$\beta = 2 \Omega_0 [A_0 B_1 - B_0 A_1] = \frac{e^{i(\theta_0 + \theta_1)}}{4 \sqrt{\mu_0 \mu_1} \Omega_0} \mathcal{D}, \quad (3-6)$$

where

$$\begin{aligned} \mathcal{C} = & (-i \Omega_0 - i \mu_0 - \gamma_0) [\dot{X}_1^* + (i \mu_1 - \gamma_1) X_1^*] \\ & - (i \Omega_0 - i \mu_0 - \gamma_0) [\dot{X}_1 + (i \mu_1 - \gamma_1) X_1], \end{aligned} \quad (3-7)$$

$$\begin{aligned} \mathcal{D} = & (-i \Omega_0 + i \mu_0 - \gamma_0) [\dot{X}_1^* + (i \mu_1 - \gamma_1) X_1^*] \\ & - (i \Omega_0 + i \mu_0 - \gamma_0) [\dot{X}_1 + (i \mu_1 - \gamma_1) X_1]. \end{aligned} \quad (3-8)$$

Now we introduce the following WKB-type expression for $X(t)$:

$$X(t) = \left(1 + i \frac{\dot{\Omega}_0}{4 \Omega_0^2}\right) \sqrt{\frac{\Omega_0}{\Omega(t)}} \mathcal{B}(t) e^{-i \Phi(t)} - i \frac{\dot{\Omega}_0}{4 \Omega_0^2} \sqrt{\frac{\Omega_0}{\Omega(t)}} \mathcal{B}(t) e^{i \Phi(t)}, \quad (3-9)$$

where

$$\Phi(t) = \int_{t_0}^t \mathcal{B}(t')^{-2} \Omega(t') dt' . \quad (3-10)$$

The correction factor $\mathcal{B}(t)$ to the WKB approximation is the solution of the differential equation

$$\frac{d^2 \mathcal{B}}{d\zeta^2} + (\Lambda + 1 - \mathcal{B}^{-4}) \mathcal{B} = 0 ; \quad \mathcal{B}(\zeta_0) = 1, \quad \frac{d\mathcal{B}}{d\zeta}(\zeta_0) = 0, \quad (3-11)$$

where

$$\zeta - \zeta_0 = \int_{t_0}^t \Omega(t') dt' , \quad (3-12)$$

and

$$\Lambda \equiv \frac{1}{4} \frac{1}{\Omega^2} \left(\frac{d\Omega}{d\zeta} \right)^2 - \frac{1}{2} \frac{1}{\Omega} \frac{d^2 \Omega}{d\zeta^2}$$

$$= \frac{5}{16} \frac{[(\Omega^2)']^2}{\Omega^6} - \frac{1}{4} \frac{(\Omega^2)''}{\Omega^4} . \quad (3-13)$$

We can prove that the solution $\mathcal{B}(t)$ of Eq.(3-11) exists in the whole range of ζ if $\Omega > 0$, therefore the expression (3-9) is valid in the whole range of t . But since its proof is lengthy and of highly mathematical nature, and since Eq.(3-11) has been fully studied in the context of the WKB approximation by many authors¹⁶⁾, we admit this fact without proof in this paper. By substituting the expression (3-9) into Eqs.(3-7) and (3-8) we obtain the final expressions:

$$\mathcal{U} = \mathcal{B}_1 \sqrt{\frac{\Omega_0}{\Omega_1}} [\mathcal{U}_1 \sin \mathcal{X}_1 + \mathcal{U}_2 \cos \mathcal{X}_1 + i(\mathcal{U}_3 \sin \mathcal{X}_1 + \mathcal{U}_4 \cos \mathcal{X}_1)], \quad (3-14)$$

$$\mathcal{V} = \mathcal{B}_1 \sqrt{\frac{\Omega_0}{\Omega_1}} [\mathcal{V}_1 \sin \mathcal{X}_1 + \mathcal{V}_2 \cos \mathcal{X}_1 + i(\mathcal{V}_3 \sin \mathcal{X}_1 + \mathcal{V}_4 \cos \mathcal{X}_1)], \quad (3-15)$$

where $\mathcal{B}_1 = \mathcal{B}(t_1)$, $\Omega_1 = \Omega(t_1)$, and $\mathcal{X}_1 = \mathcal{X}(t_1)$, and

$$\mathcal{U}_1 = 2(\mu_1 \gamma_0 + \mu_0 \gamma_1) + \mu_1 \frac{\dot{\Omega}_0}{\Omega_0} + \mu_0 \frac{\dot{\Omega}_1}{\Omega_1} + 2\mu_0 \frac{\dot{\mathcal{B}}_1}{\mathcal{B}_1}, \quad (3-16)$$

$$\mathcal{U}_2 = 2(\mu_1 \Omega_0 - \mu_0 \Omega_1 \mathcal{B}_1^{-2}), \quad (3-17)$$

$$\begin{aligned} \mathcal{U}_3 = & 2(\Omega_0 \Omega_1 \mathcal{B}_1^{-2} - \mu_0 \mu_1) + \frac{1}{2} \frac{\dot{\Omega}_0}{\Omega_0} \frac{\dot{\Omega}_1}{\Omega_1} + \gamma_0 \frac{\dot{\Omega}_1}{\Omega_1} + \gamma_1 \frac{\dot{\Omega}_0}{\Omega_0} \\ & + 2\gamma_0 \gamma_1 - \frac{\dot{\mathcal{B}}_1}{\mathcal{B}_1} \left(\frac{\dot{\Omega}_0}{\Omega_0} + 2\gamma_0 \right), \end{aligned} \quad (3-18)$$

$$\mathcal{U}_4 = \Omega_0 \frac{\dot{\Omega}_1}{\Omega_1} - \Omega_1 \frac{\dot{\Omega}_0}{\Omega_0} \mathcal{B}_1^{-2} + 2(\Omega_0 \gamma_1 - \gamma_0 \Omega_1 \mathcal{B}_1^{-2}) - 2\Omega_0 \frac{\dot{\mathcal{B}}_1}{\mathcal{B}_1}, \quad (3-19)$$

and the expressions for \mathcal{C}_1 ($l=1\sim 4$) are obtained by the replacement $\mu_0 \rightarrow -\mu_0$ in those for \mathcal{D}_1 .

4. Constraints Imposed by the Implementability Condition of the Bogoliubov Transformation.

Now in this section we study the asymptotic behavior of \mathcal{B} for large k and from this we derive constraints on μ and γ imposed by the implementability condition of the Bogoliubov transformation. Since in the usual WKB approximation $\mathcal{B} \approx 1$, we change the variable from \mathcal{B} to $u = \mathcal{B} - 1$. Then Eq.(3-11) is written as

$$\frac{d^2 u}{d\zeta^2} + 4u = -(1+u)\Lambda - u g(u), \quad (4-1)$$

where

$$g(u) = \frac{u(3u^2 + 8u + 6)}{(1+u)^3}, \quad (4-2)$$

and the initial condition is

$$u(\zeta_0) = 0, \quad \frac{du}{d\zeta}(\zeta_0) = 0. \quad (4-3)$$

With the aid of the Green's function of the differential operator $d^2/d\zeta^2 + 4$, Eq.(4-1) can be transformed to the integral equation

$$u(\zeta) = -\frac{1}{2} \int_{\zeta_0}^{\zeta} \sin(2\zeta - 2\zeta') [(1+u(\zeta'))\Lambda(\zeta') + u(\zeta')g(u(\zeta'))] d\zeta'. \quad (4-4)$$

Returning to the original time variable t , we obtain

$$u(t) = -\frac{1}{2} \int_{t_0}^t \sin \left(2 \int_{t'}^t \Omega(t'') dt'' \right) \left[(1 + u(t')) \Lambda(t') + u(t') g(u(t')) \right] \Omega(t') dt', \quad (4-5)$$

and

$$\dot{u}(t) = -\Omega(t) \int_{t_0}^t \cos \left(2 \int_{t'}^t \Omega(t'') dt'' \right) \left[(1 + u(t')) \Lambda(t') + u(t') g(u(t')) \right] \Omega(t') dt'. \quad (4-6)$$

Now we will derive the estimations of $u(t)$ and $\dot{u}(t)$ by $\Lambda(t)$ from Eqs. (4-5) and (4-6). Let $\lambda(t)$ be the maximum value of $|u(t')|$ for $t_0 \leq t' \leq t$, and t_* be the maximum value of t , such that

$$\int_{t_0}^t |g(u(t'))| \Omega(t') dt' \leq 1, \quad (4-7)$$

and

$$\int_{t_0}^t |\Lambda(t')| \Omega(t') dt' \leq \frac{1}{2}. \quad (4-8)$$

Then from Eq. (4-5), we obtain the inequality for $t_0 \leq t \leq t_*$

$$|u(t)| \leq \frac{1}{2} (1 + \lambda(t)) \int_{t_0}^t |\Lambda(t')| \Omega(t') dt' + \frac{1}{2} \lambda(t). \quad (4-9)$$

Since the right-hand side of Eq. (4-9) is a monotonically increasing function of t , we can replace $|u(t)|$ by $\lambda(t)$ in this equation. By solving it with respect to $\lambda(t)$, we obtain for $t_0 \leq t \leq t_*$

$$\lambda(t) \leq 2 \int_{t_0}^t |\Lambda(t')| \Omega(t') dt'. \quad (4-10)$$

Here suppose that t_* remained finite as $|\Lambda(t)|\Omega(t)$ and $|\Lambda(t)|\Omega(t)^2$ converge to zero locally uniformly. Then from Eq.(4-10) and the definition of $g(u)$, the left-hand sides of Eqs. (4-7) and (4-8) both tend to zero even for $t=t_*$, leading to the contradiction to the definition of t_* . Therefore, for any $t_1 (>t_0)$, Eq.(4-10) is valid in $t_0 \leq t \leq t_1$ if $|\Lambda(t)|\Omega(t)$ and $|\Lambda(t)|\Omega(t)^2$ is sufficiently small uniformly in this range. Thus we obtain the estimate

$$|u(t)| \leq 2 \int_{t_0}^t |\Lambda(t')| \Omega(t') dt', \quad (4-11)$$

which is valid for any $t(>t_0)$ under the same condition. A similar estimate for $\dot{u}(t)$ can be obtained from this. Using conditions (4-7) and (4-8), and noting that $|u(t)| \leq 1$ from Eq.(4-11) under these conditions, Eq.(4-6) yields the estimate

$$|\dot{u}(t)| \leq 4 \Omega(t) \int_{t_0}^t |\Lambda(t')| \Omega(t') dt'. \quad (4-12)$$

If $\ddot{\Omega}$ exists, we can obtain finer estimations. By partial integration Eqs.(4-5) and (4-6) are written as

$$\begin{aligned} u(t) = & -\frac{1}{4} [\Lambda(t)(1+u(t)) + u(t)g(u(t))] + \frac{1}{4} \Lambda(t) \cos(2 \int_{t_0}^t \Omega(t') dt') \\ & + \frac{1}{4} \int_{t_0}^t \cos(2 \int_{t'}^t \Omega(t'') dt'') \frac{d}{dt'} [\Lambda(1+u) + u g(u)] dt', \end{aligned} \quad (4-13)$$

and

$$\dot{u}(t) = -\frac{1}{2} \Omega(t) \Lambda(t) \sin(2 \int_{t_0}^t \Omega(t') dt')$$

$$+ \frac{1}{2} \Omega(t) \int_{t_0}^t \sin \left(2 \int_{t'}^t \Omega(t'') dt'' \right) \frac{d}{dt'} \left[\Lambda(1+u) + u g(u) \right] dt'. \quad (4-14)$$

Using Eqs.(4-7), (4-8), (4-11) and (4-12), Eqs.(4-13) and (4-14) yield the estimates

$$|u(t)| \leq \frac{1}{2} |\Lambda(t)| + \frac{1}{4} |\Lambda(t_0)| + \frac{1}{2} \int_{t_0}^t |\dot{\Lambda}(t')| dt' \\ + (P + Q \int_{t_0}^t \Omega(t') dt') \left[\int_{t_0}^t |\Lambda(t')| \Omega(t') dt' \right]^2, \quad (4-15)$$

and

$$|\dot{u}(t)| \leq \frac{1}{2} \Omega(t) |\Lambda(t)| + \Omega(t) \int_{t_0}^t |\dot{\Lambda}(t')| dt' \\ + \Omega(t) \left(S + T \int_{t_0}^t \Omega(t') dt' \right) \left[\int_{t_0}^t |\Lambda(t')| \Omega(t') dt' \right]^2, \quad (4-16)$$

where P, Q, S and T are some positive constants.

These estimates enable us to obtain the asymptotic behavior of \mathcal{B} for large k. From Eqs.(2-8) and (3-13) we obtain

$$\Lambda \sim O(k^{-4}) \quad \text{locally uniformly w.r.t. } t. \quad (4-17)$$

Hence Eqs.(4-11) and (4-12) yield the estimates

$$|\mathcal{B}(t) - 1| \sim O(k^{-3}), \quad (4-18)$$

$$|\dot{\mathcal{B}}(t)| \sim O(k^{-2}). \quad (4-19)$$

If $\ddot{\Omega}$ exists, Eqs.(4-15) and (4-16) give finer estimates

$$|\mathcal{B}(t) - 1| \sim O(k^{-4}), \quad (4-20)$$

$$|\dot{\mathcal{B}}(t)| \sim O(k^{-3}). \quad (4-21)$$

Now we apply these estimations to the study of the implementability condition of the Bogoliubov transformation. From Eq.(3-6) the condition (2-23) is expressed as

$$\int^{+\infty} \frac{dk k^2}{\mu_0 \mu_1 \Omega_0^2} |\mathcal{D}|^2 \sim \int^{+\infty} \frac{dk}{\mu^2} |\mathcal{D}|^2 < +\infty \quad (4-22)$$

Recalling the assumption on the monotonic dependence of μ and γ on k for large k , this condition can be written as

$$\int^{+\infty} \frac{dk}{\mu^2} |\mathcal{D}_l|^2 < +\infty \quad (l=1 \sim 4) . \quad (4-23)$$

Note that $\dot{\Omega}/\Omega$ and $\dot{\mathcal{B}}/\mathcal{B}$ are of order $O(k^{-2})$ from Eqs. (2-8), (4-20) and (4-21). From this, if $\gamma \sim O(k^{-2})$, then $|\mathcal{D}_1|^2 / \mu^2 \sim O(k^{-2})$, and if γ grows faster than k^{-2} as $k \rightarrow \infty$, $|\mathcal{D}_1|^2 / \mu^2 \sim 4 \gamma^2$. Hence the condition (4-23) for $l=1$ requires

$$\gamma \sim o(k^{-1/2}) . \quad (4-24)$$

Then from Eqs. (3-18) and (4-18) we obtain

$$\mathcal{D}_3 = 2(\Omega_0 \Omega_1 - \mu_0 \mu_1) + O(k^{-1}) . \quad (4-25)$$

First suppose that $\mu \sim o(k)$. Then Eq. (4-25) yields $\mathcal{D}_3 \sim O(k^2)$, hence $|\mathcal{D}_3|^2 / \mu^2 \sim 4k^4 / \mu^2$, which grows faster than k^2 . Next suppose that μ grows faster than k . Then $\mathcal{D}_3 \sim -2\mu^2$. Hence $|\mathcal{D}_3|^2 / \mu^2 \sim 4\mu^2$, which grows faster than k^2 . Therefore condition (4-23) for $l=3$ requires that $\mu = \mu_* k + o(k)$ with some positive constant μ_* . Then the condition for \mathcal{D}_3 can be

written as

$$|\mathcal{D}_3| \sim o(k^{-\frac{1}{2}}) . \quad (4-26)$$

By rewriting the first term in Eq.(4-25) as

$$\Omega_0 \Omega_1 - \mu_0 \mu_1 = \Omega_0^2 - \mu_0^2 + \frac{\mu_0}{\mu_0 + \mu_1} (\mu_0^2 - \mu_1^2) + \frac{\Omega_0}{\Omega_0 + \Omega_1} (\Omega_1^2 - \Omega_0^2) ,$$

and noting that the last term in this equation is of order $O(1)$, we can easily see that condition (4-26) requires

$$\mu^2 = \Omega^2 + o(k^{\frac{1}{2}}) \quad (4-27)$$

With Eqs.(4-24) and (4-27), all the conditions (4-23) are satisfied, and these are the constraints we wanted to obtain.

In concluding this section we remark on a special case. Among various choices of the particle-defining modes, that which diagonalizes the Hamiltonian at each cosmic time is the most natural one. For this choice we can derive an interesting fact from the result obtained in this section. As will be shown in the next section, for the Hamiltonian diagonalizing modes, $Y = (1 - \xi) R^{-1} \dot{R}$. Then condition (4-24) requires that $\xi = 1$ unless $R_0^{-1} \dot{R}_0$ and $R_1^{-1} \dot{R}_1$ are both zero. Therefore we can conclude that the coupling of a scalar field with the background geometry must be conformal in order that the Bogoliubov transformation between two Fock representations at different times specified by the simultaneous Hamiltonian diagonalization condition is implementable.

5. Constraints Imposed by the Energy Generation Rate

The constraints on μ and γ obtained in § 4 from the implementability condition of the Bogoliubov transformation are rather weak ones in general. In this section we show that stronger constraints are obtained if we turn our attention to the energy generation rate. For the scalar field in a spatially homogeneous and isotropic universe we define the Hamiltonian by

$$H(\tau) = -R^4(\tau) \int_{t=\tau} dV T^t_t, \quad (5-1)$$

where T^μ_ν are the mixed components of the energy-momentum tensor. Then the difference of the vacuum expectation values of $H(t_1)$ at $t=t_0$ and t_1 ,

$$\Delta\mathcal{E} \equiv \langle \mathcal{V}_{t_0} | H(t_1) | \mathcal{V}_{t_0} \rangle - \langle \mathcal{V}_{t_1} | H(t_1) | \mathcal{V}_{t_1} \rangle, \quad (5-2)$$

which is referred to as energy generation rate in this paper, should be finite if we restrict the field in a finite volume, though H itself is a divergent quantity.^{8),9)} This is the second requirement, which we consider in this section.

The energy-momentum tensor of a scalar field ϕ in a background geometry $g_{\mu\nu}$ is given by ⁸⁾

$$T_{\mu\nu} \equiv -\frac{2}{\sqrt{-g}} \frac{\delta}{\delta g^{\mu\nu}} \int d^4x \mathcal{L}$$

$$= \partial_\mu \phi \partial_\nu \phi - \frac{1}{2} g_{\mu\nu} \partial_\sigma \phi \partial^\sigma \phi - \frac{1}{2} g_{\mu\nu} m^2 \phi^2 + \frac{\xi}{6} [G_{\mu\nu} \phi^2 + g_{\mu\nu} \nabla_\sigma \phi \nabla^\sigma \phi - \nabla_\mu \nabla_\nu (\phi^2)], \quad (5-3)$$

Where $G_{\mu\nu} = R_{\mu\nu} - 1/2 g_{\mu\nu} R$ is the Einstein tensor, and ∇_μ denotes the covariant differentiation with respect to the coordinates x^μ . By substituting the expression (2-9) into Eq. (5-3) and using Eqs. (2-6), (2-12), and (2-13), Eq. (5-1) yields

$$H(\tau) = \frac{1}{2} \sum_{(k)} \left\{ [\tilde{\omega}^2 + (-i\mu + \gamma + (\xi-1)R^{-1}\dot{R})^2]_\tau f_{k(\tau)}^2 a_\tau[(k)] a_\tau[-(k)] + [\tilde{\omega}^2 + (i\mu + \gamma + (\xi-1)R^{-1}\dot{R})^2]_\tau f_{k(\tau)}^{*2} a_\tau[(k)]^\dagger a_\tau[-(k)]^\dagger + \frac{1}{2\mu(\tau)} [\tilde{\omega}^2 + \mu^2 + (\gamma + (\xi-1)R^{-1}\dot{R})^2]_\tau (2 a_\tau[(k)]^\dagger a_\tau[(k)] + 1) \right\}, \quad (5-4)$$

where

$$\tilde{\omega}^2 = k^2 + m^2 R^2 + \xi \chi, \quad (5-5)$$

and the subscript τ in the right-hand sides of the square brackets means that the values estimated at $t=\tau$ should be taken. By virtue of the equation $X(t)\dot{X}^*(t) - X^*(t)\dot{X}(t) = 2i\Omega_0$ obtained from Eqs. (2-7) and (3-1), and Eqs. (3-2), (3-3), and (3-4), we can easily show that

$$\{f_{(t_1)}(t_1)\}^2 = - \frac{e^{2i\theta_1}}{2\mu_1}. \quad (5-6)$$

From Eqs. (2-10), (2-16), (2-17), (3-5), (3-6), and (5-6),

$\Delta \mathcal{E}$ is written as

$$\Delta \mathcal{E} = \sum_{(k)} \frac{\mathcal{K}}{32 \mu_0 \mu_1^2 \Omega_0^2} , \quad (5-7)$$

$$\begin{aligned} \mathcal{K} = & [\tilde{\omega}_1^2 - \mu_1^2 + (\gamma_1 + (\xi-1) R_1^{-1} \dot{R}_1)^2] \mathcal{R}_e [\mathcal{C} \mathcal{D}] \\ & - 2 \mu_1 (\gamma_1 + (\xi-1) R_1^{-1} \dot{R}_1) \mathcal{I}_m [\mathcal{C} \mathcal{D}] \\ & + [\tilde{\omega}_1^2 + \mu_1^2 + (\gamma_1 + (\xi-1) R_1^{-1} \dot{R}_1)^2] |\mathcal{D}|^2 , \end{aligned} \quad (5-8)$$

where the subscript 0 and 1 denote the values estimated at $t=t_0$ and t_1 , respectively, as in the previous sections, and \mathcal{R}_e and \mathcal{I}_m mean to take the real and the imaginary part of the subsequent quantity, respectively. By the same reason as in the argument on the implementability condition of the Bogoliubov transformation, the finiteness condition for $\Delta \mathcal{E}$ can be written as

$$\left| \int_0^{+\infty} dk \frac{k^2}{\mu_0 \mu_1^2 \Omega_0^2} \mathcal{K} \right| < +\infty . \quad (5-9)$$

With the aid of Eqs.(2-8), (4-20), (4-21), (4-24), and (4-27), and the estimates, $\mu_1 \Omega_0 + \mu_0 \Omega_1 = 2 \Omega_0^2 + o(k^{1/2})$ and $\Omega_0 \Omega_1 + \mu_0 \mu_1 = 2 \Omega_0^2 + o(k^{1/2})$, we obtain, from Eqs. (3-16)~(3-19) and the corresponding equations for \mathcal{C}_1 ,

$$\mathcal{C}_1 = 2(\gamma_0 \mu_1 - \gamma_1 \mu_0) + O(k^{-1}) , \quad (5-10)$$

$$\mathcal{C}_2 = 2 \Omega_0^2 + o(k^{1/2}) , \quad (5-11)$$

$$\mathcal{L}_3 = 2 \Omega_0^2 + o(k^{1/2}) , \quad (5-12)$$

$$\mathcal{L}_4 = 2(\Omega_0 \gamma_1 - \Omega_1 \gamma_0) + o(k^{-1}) , \quad (5-13)$$

and

$$\mathcal{D}_1 = 2(\gamma_0 \mu_1 + \gamma_1 \mu_0) + \mu_1 \Omega_0^{-1} \dot{\Omega}_0 + \mu_0 \Omega_1^{-1} \dot{\Omega}_1 + o(k^{-2}) , \quad (5-14)$$

$$\mathcal{D}_2 = 2(\Omega_0 \mu_1 - \Omega_1 \mu_0) + o(k^{-2}) , \quad (5-15)$$

$$\mathcal{D}_3 = 2(\Omega_0 \Omega_1 - \mu_0 \mu_1) + o(k^{-1}) , \quad (5-16)$$

$$\mathcal{D}_4 = 2(\Omega_0 \gamma_1 - \gamma_0 \Omega_1) + \Omega_0 \Omega_1^{-1} \dot{\Omega}_1 - \Omega_1 \Omega_0^{-1} \dot{\Omega}_0 + o(k^{-1}) . \quad (5-17)$$

Substituting Eqs.(5-10)~(5-17) into Eq.(5-8) and noting that $\Omega_1^{-1} \Omega_0 \Omega^2 = 1 + o(k^{-2})$ from Eq.(2-8) and (4-20), we obtain

$$\begin{aligned} \mathcal{K} = & 4 \Omega_0^2 (\tilde{\omega}_1^2 - \mu_1^2 + (1-\xi) R_1^{-2} \dot{R}_1^2) \{ \mu_1^2 - \Omega_1^2 \\ & + (\Omega_0^2 - \mu_0^2) \cos 2\Phi_1 + 2 \gamma_0 \Omega_0 \sin 2\Phi_1 \} \\ & - 8 \mu_1 \Omega_0^2 (\gamma_1 + (\xi-1) R_1^{-1} \dot{R}_1) \{ 2 \Omega_0 \gamma_1 + \Omega_0 \Omega_1^{-1} \dot{\Omega}_1 \\ & - (2 \Omega_0 \gamma_0 + \Omega_1 \Omega_0^{-1} \dot{\Omega}_0) \cos 2\Phi_1 + (\Omega_0^2 - \mu_0^2) \sin 2\Phi_1 \} \\ & + 2 \Omega_0^2 [4(\gamma_0^2 + \gamma_1^2) \Omega_0^2 + (\mu_0^2 - \Omega_0^2)^2 + (\mu_1^2 - \Omega_1^2)^2 \\ & + 2 \{ -4 \gamma_0 \gamma_1 \Omega_0^2 + (\Omega_0^2 - \mu_0^2)(\mu_1^2 - \Omega_1^2) \} \cos 2\Phi_1 \\ & + 4 \Omega_0 \{ \gamma_1 (\Omega_0^2 - \mu_0^2) + \gamma_0 (\mu_1^2 - \Omega_1^2) \} \sin 2\Phi_1] \\ & + o(k^2) . \end{aligned} \quad (5-18)$$

Since from Eqs.(2-8) and (4-20) Φ_1 has the asymptotic behavior

$$\Phi_1 = \int_{t_0}^{t_1} \beta(t)^{-2} \Omega(t) dt = k(t_1 - t_0) + O(k^{-1}), \quad (5-19)$$

recalling the assumption on the monotonic behavior of μ and γ for large k , terms of the form $o(k^3) \times \sin 2\Phi_1$ (or $\cos 2\Phi_1$) in Eq.(5-8) make finite contributions in the integral in Eq.(5-9). Therefore, discarding the terms which make finite contributions in the integral, we obtain

$$\begin{aligned} \mathcal{K} \sim & 4\Omega_0^2(\mu_1^2 - \Omega_1^2) \{ \tilde{\omega}_1^2 - \mu_1^2 + (1-\xi) R_1^{-2} \dot{R}_1^2 \} \\ & - 8\Omega_0^2 \mu_1 (\xi-1) R_1^{-1} \dot{R}_1 \{ 2\Omega_0 \gamma_1 + \Omega_0 \Omega_1^{-1} \dot{\Omega}_1 \\ & - 2\gamma_0 \Omega_0 \cos 2\Phi_1 + (\Omega_0^2 - \mu_0^2) \sin 2\Phi_1 \} \\ & + 2\Omega_0^2 \{ 4(\gamma_0^2 - \gamma_1^2) \Omega_0^2 + (\mu_0^2 - \Omega_0^2)^2 \\ & + (\mu_1^2 - \Omega_1^2)^2 \} \quad . \end{aligned} \quad (5-20)$$

Now let us examine what constraints are imposed on μ and γ by condition (5-9). First we will consider the case $\xi=0$, i.e., the minimal coupling case. Since in this case all the terms other than $-16(\xi-1)R_1^{-1}\dot{R}_1\Omega_0^3\mu_1\gamma_1$ in Eq.(5-20) are of order $o(k^3)$, condition (5-9) requires $\Omega_0^3\mu_1\gamma_1 \sim o(k^3)$, hence

$$\gamma \sim o(k^{-1}) \quad . \quad (5-21)$$

Furthermore in order that the contribution from the oscillatory terms is finite, it should be that $\Omega_0^2 \mu_1 (\Omega_0^2 - \mu_0^2) \sim o(k^3)$, hence

$$\mu^2 = \Omega^2 + o(1) \quad . \quad (5-22)$$

Under the conditions (5-21) and (5-22), condition (5-9) is equivalent to the condition $\Omega_0^2 \mu_1 (2\Omega_0 \gamma_1 + \Omega_0 \Omega_1^{-1} \dot{\Omega}_1) \sim o(k^2)$, hence

$$\gamma = -\frac{1}{2} \Omega^{-1} \dot{\Omega} + o(k^{-2}) \quad . \quad (5-23)$$

Next we consider the case $\xi=1$, i.e., the conformal coupling case. In this case, Eq.(5-20) reduces to

$$\mathcal{K} \sim 2 \tilde{\omega}_0^2 \{ (\mu_0^2 - \tilde{\omega}_0^2)^2 - (\mu_1^2 - \tilde{\omega}_1^2)^2 + 4 \tilde{\omega}_0^2 (\gamma_0^2 - \gamma_1^2) \} \quad (5-24)$$

Therefore condition (5-9) is equivalent to the condition

$$\Delta [(\mu^2 - \tilde{\omega}^2)^2 + 4 \tilde{\omega}^2 \gamma^2] \sim o(1) \quad , \quad (5-25)$$

where Δ means to take the difference of the values estimated at two different times. In summary, for the minimal coupling case, the requirement that the energy generation rate is finite yields very strong constraints on μ and γ and they are completely determined by Ω in large- k region in essence. In contrast, for the conformal coupling case, only a rather weak constraint (5-25) is imposed.

Finally we will remark on the special case in which the particle-defining modes are specified by the simultaneous Hamiltonian diagonalization condition. From Eq.(5-3) this case is characterized by

$$\mu = \tilde{\omega} \quad , \quad \gamma = (1-\xi) R^{-1} \dot{R} \quad . \quad (5-26)$$

In this case, as was shown in §4, the implementability condition of the Bogoliubov transformation requires that $\xi = 1$. Therefore condition (5-25) is satisfied. Since for the Hamiltonian diagonalizing modes, the normal-ordered Hamiltonian with respect to these modes at each time is always finite and positive definite, $\Delta \mathcal{E}$ can be said to mean the energy generation rate on its proper sense. Hence we can say that for the Hamiltonian diagonalizing Fock representations and the conformal coupling, the energy generation rate remains finite as well as the Bogoliubov transformation is implementable.

6. Concluding Remarks

In this paper we studied on the freedom in assigning Fock representations to each cosmic time for a free neutral scalar field in spatially homogeneous and isotropic universes. We made this assignment by specifying the particle-defining modes at each time with the aid of two functions, $\mu_k(t)$ and $\gamma_k(t)$. In

order to obtain constraints on $\mu_k(t)$ and $\gamma_k(t)$, we considered two requirements. The first of them, the implementability condition of the Bogoliubov transformation imposed rather weak constraints, but the second requirement that the energy generation rate per unit volume should be finite yielded strong constraints on the large- k asymptotic behavior of $\mu_k(t)$ and $\gamma_k(t)$. Especially for the minimal coupling case, $\mu_k(t)$ and $\gamma_k(t)$ were, in essence, completely determined by the mode frequency $\Omega(t)$ in the large- k region.

Here we comment on the work of Fulling.¹⁷⁾ He examined whether the unitarity condition (2-23) is satisfied or not for modes suggested by the first-order WKB approximation for the field equation in the generalized Kasner universe. When restricted to the isotropic case, the modes he examined in detail correspond to those given by $\mu = \Omega$ and $\gamma = 0$ in our notation. Of course he also dealt with some more general cases in connection with the canonical Hamiltonian diagonalizing modes, but in these cases his consideration remained rather rough one. By using our results his conclusion on these cases can be also justified exactly. Next we refer to technical aspects. Since his argument was based on the estimation of the direct difference of the WKB approximation from the exact solution, it was difficult to obtain the information on the phase of the error. In contrast, in our method, since we confined the correction for the WKB approximation to a single

real function \mathcal{B} , we could explicitly distinguish the correction to the amplitude from that to the phase, which enabled us to obtain the delicate constraints on μ and γ .

In general our consideration does not give informations on the small- k behavior of $\mu_k(t)$ and $\gamma_k(t)$. In order to determine $\mu_k(t)$ and $\gamma_k(t)$ in the full range of k , more deeper physical considerations should be needed. But in the cases where the particle defining modes are determined by other physical grounds, our results give an important criterion on their acceptability. In fact, especially for the simultaneous Hamiltonian diagonalizing modes, we showed that the coupling of a free neutral scalar field with the background geometry should be conformal in order that the Bogoliubov transformation between Fock representations at different times is implementable. Since, for the high frequency modes, the assumption on the locality of the definition of the particle-defining modes might be reasonable, and the positive definiteness of the Hamiltonian might be also required, physically acceptable Fock representations will diagonalize the Hamiltonian in the large- k region. Therefore, the fact stated above seem to suggest that scalar fields should interact with the background geometry through conformal coupling.

Finally we remark on the extent to which our consideration is valid. Our consideration crucially depend on the quasi-adiabatic nature of the definition of particle modes and the

validity of the WKB-type expression (3-9). Especially near the cosmic singularity these assumptions may break down. In such a region non-local characterization of field states may be necessary. Assumption on the isotropy of universes also seems to have played an important role. In fact Fulling has shown that anisotropy brings in a new serious difficulty to the consideration of the unitarity condition.¹⁷⁾ These problems remain to be solved in the future.

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